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06/12/12

6 Jun 12
15N - 16N

Advanced Reaction Engineering

Time Dependent operations

Catalyst Deactivation

(a) (b) (c)

$C_2H_2 + HCl = C_2H_3Cl$

(g) (g) Vcl

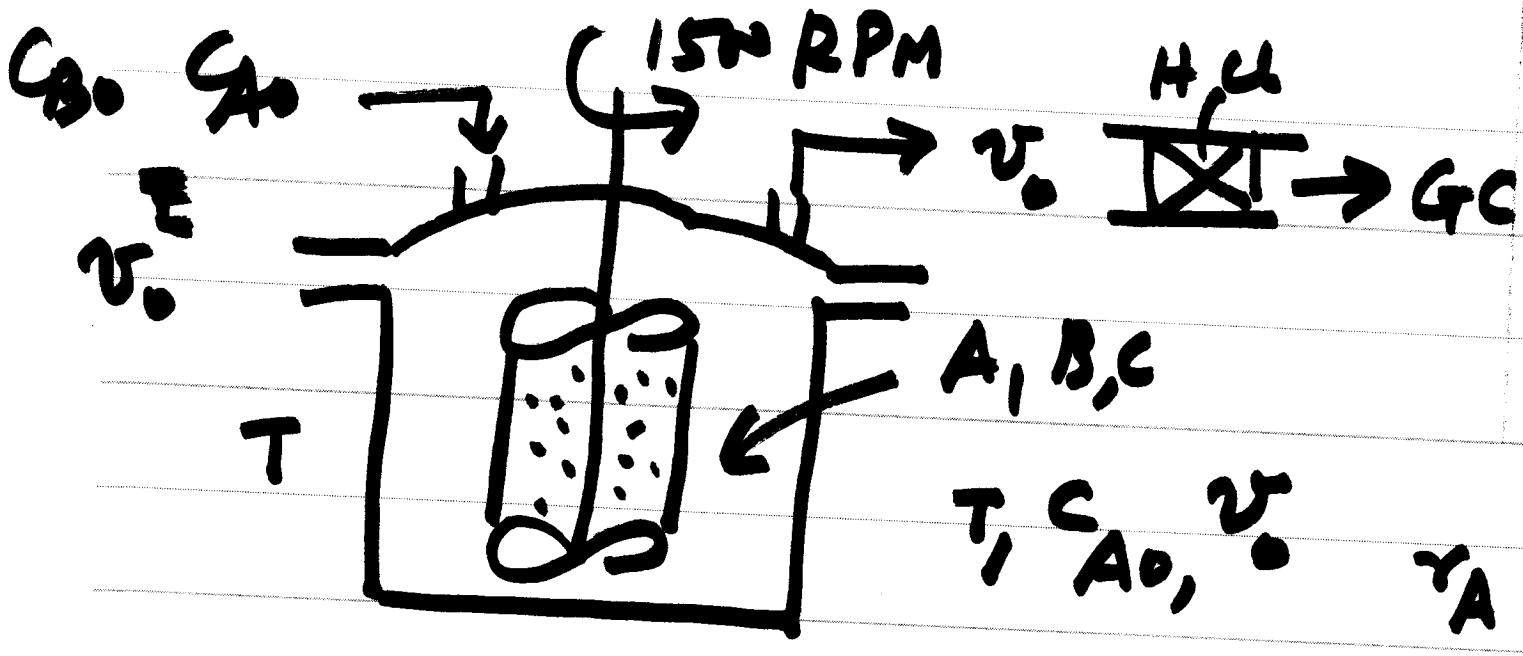
10 % $\frac{w}{w}$ $HgCl_2$ Catalyst / supported on activated Carbon

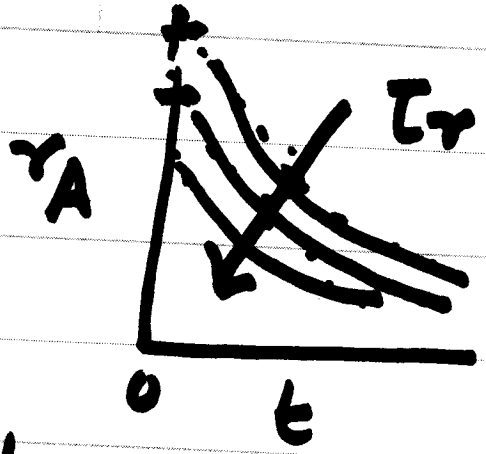
Determination of Deactivation kinetics.

$$r_d = k_d a^m C_A^p C_B^q C_C^r$$

k_d, m, p, q, r are parameters of deactivation rate function.

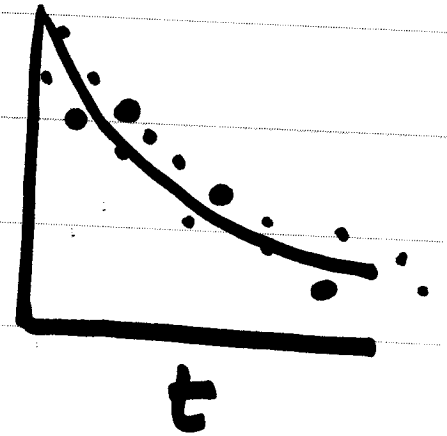
$$-\frac{da}{dt} = r_d = k_d(T)\, a^m C_A^p C_B^q C_C^r$$





Stirred Basket Reactor

$$a = \left[\frac{r_A(t)}{r_A(0)}\right]$$



$T = 180\,c$

$A = HCl$

SN	y_{A0}	t (hr)	$a = \frac{r(t)}{r(0)}$	F_{t0} mol/min
1	0.12	0.0	1.0	0.078
2	0.28	2.5	0.86	0.032
3	0.39	12.5	0.63	0.023
4	0.28	14.0	0.56	0.032
5	0.22	17.0	0.41	0.041
6	0.17	25.0	0.36	0.051
7	0.22	38.2	0.24	0.041

y_{A0} = mol. Fraction HCl (A)

$P_t = 1$ atm.

T : 180 c

$$a = \frac{r(t)}{r(0)}.$$

5/1

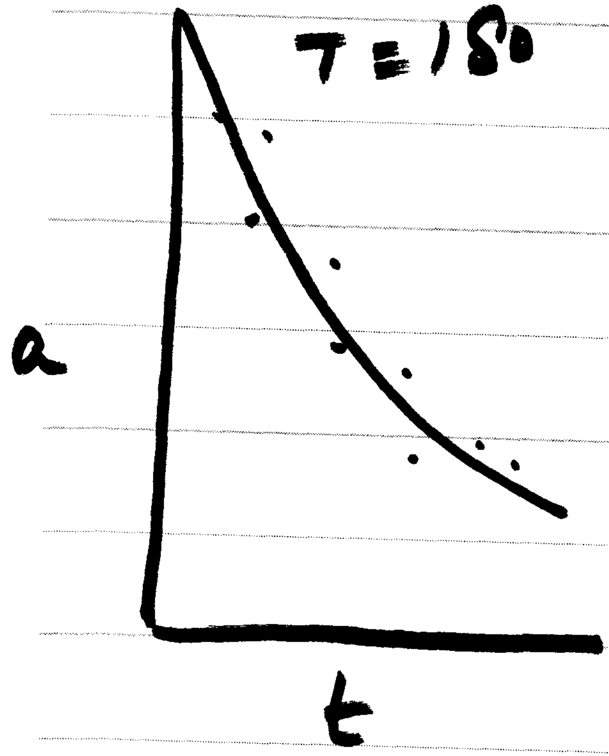
T = 210

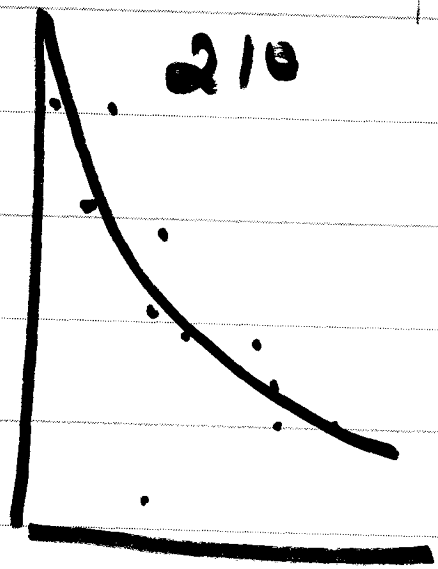
mol/min

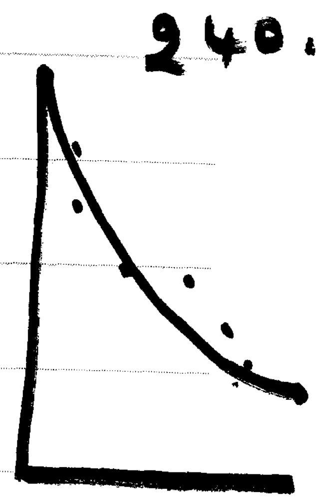
SN	y_{A0}	F_{t0}	θ_t	a
1	0.12	0.034	0.0	1.0
2	0.28	0.032	0.4	0.96
3	0.39	0.023	10.2	0.35
4	0.28	0.032	3.4	0.70
5	0.22	0.041	10.8	0.32
6	0.17	0.051	7.9	0.43
7	0.22	0.041	15.8	0.19

T = 240 c

SN	y_{to}	F_{to}	a	t	a
1	0.12	0.071	0		1.0
2	0.28	0.032	0.9		0.84
3	0.39	0.028	1.9		0.12
4	0.28	0.032	5.8		0.30
5	0.22	0.041	3.8		0.41
6	0.12	0.051	1.5		0.74
7	0.22	0.041	0.6		0.86





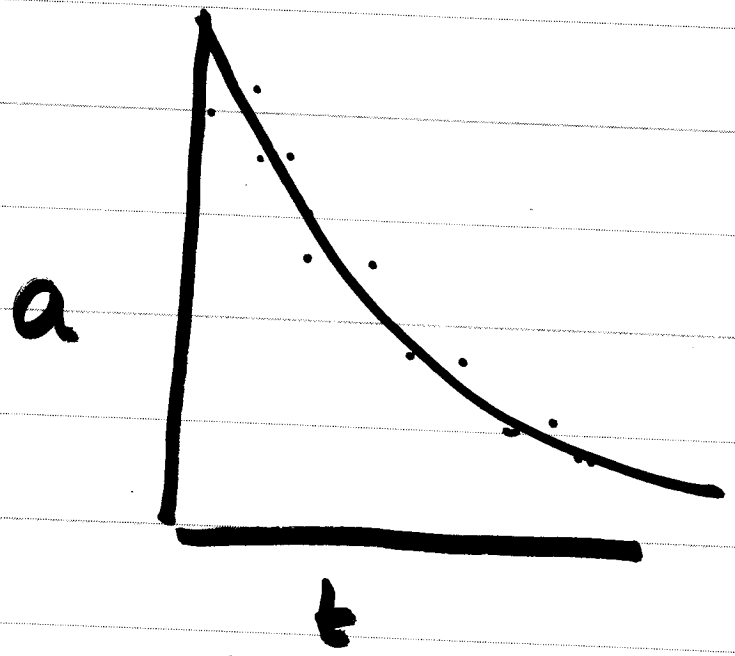


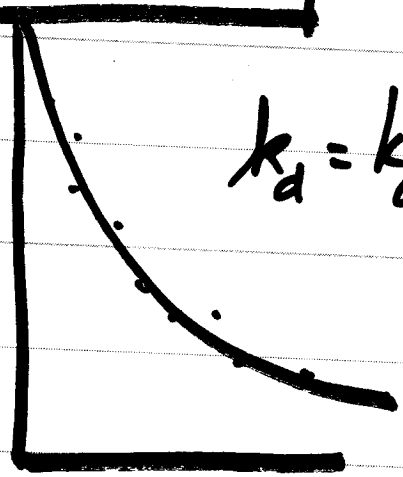
(1) In this data concentration dependence of activity seems to be very small or p, q and r = 0

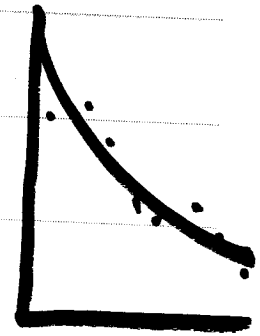
$$-\frac{da}{dt} = k_d a^m \cancel{q_A q_B q_C}$$

$$a = e^{-k_d t}$$

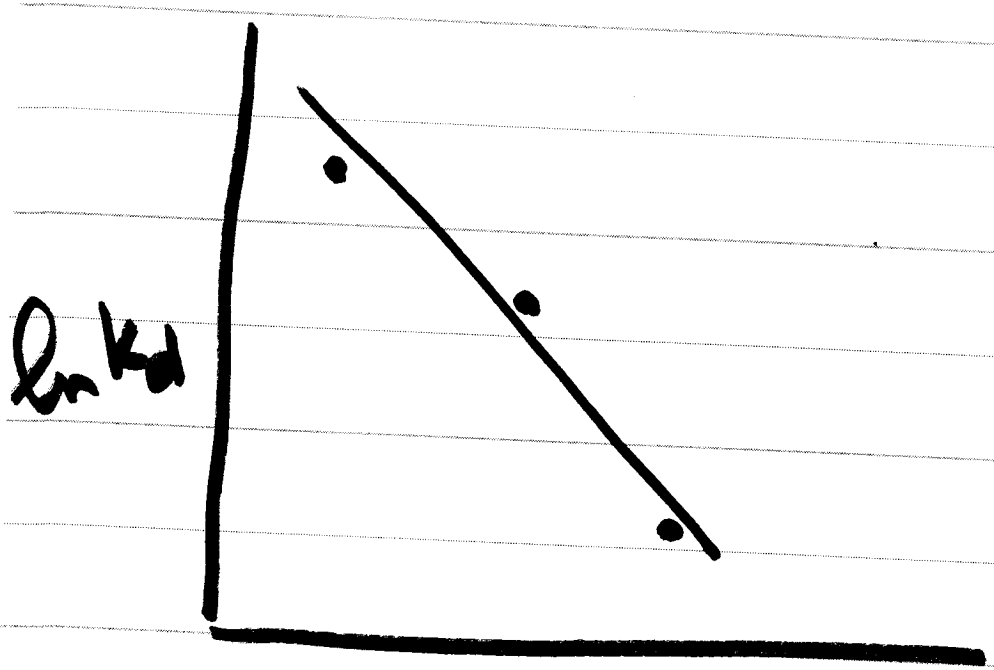
$$k_d = k_{d0} e^{-E_d/RT}$$







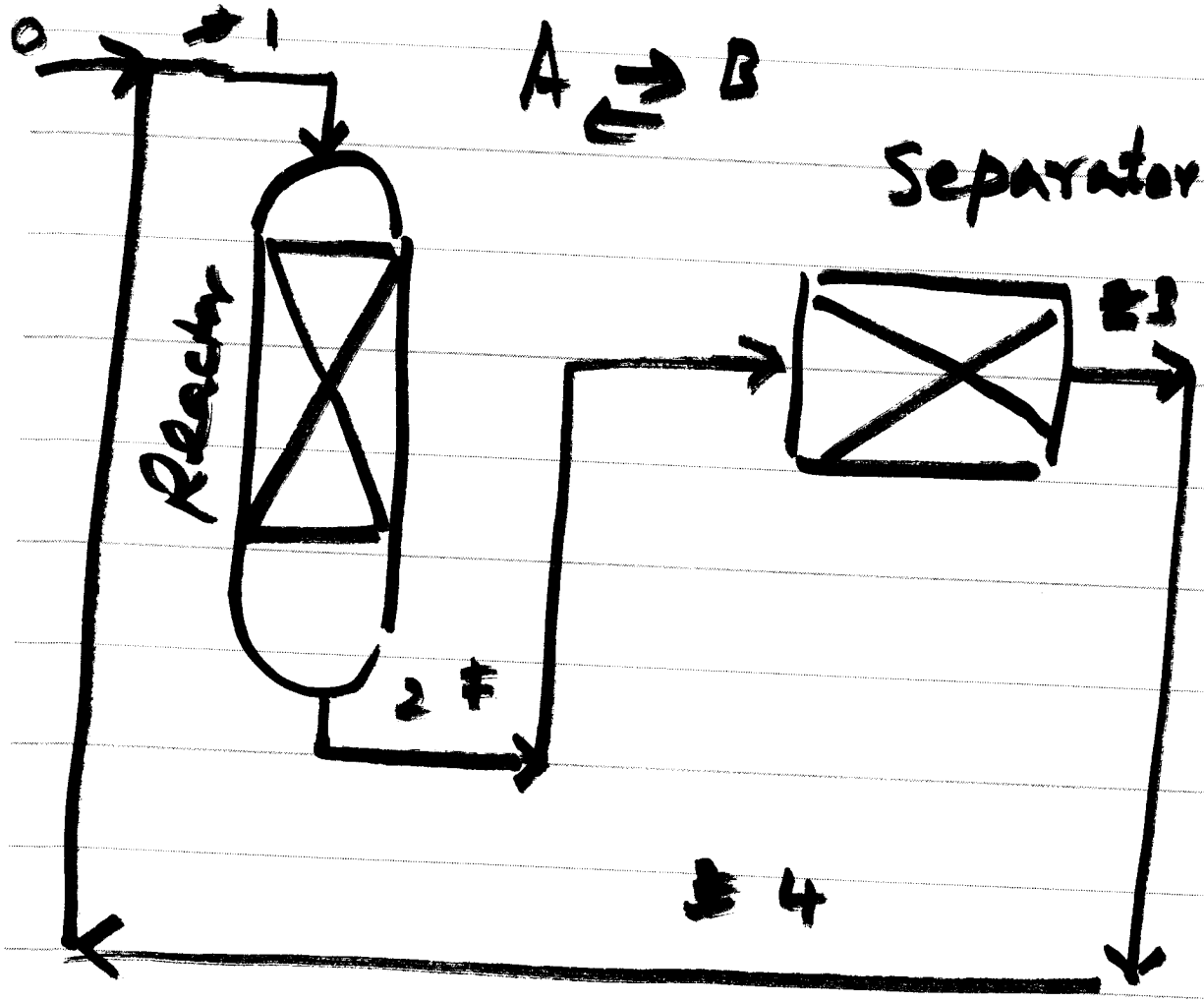
q_t is observed that exponent $m \cong 1$



slope $= -E_d/R =$

$E_d \simeq$ 10,000 Cal/mol.

1°



$$h = e^{8.8 - \frac{500}{T}}$$

$$k_1 = 2 \times 10^{13 - \frac{2500}{T}}$$

$$K = \exp\left[-19.5 + \frac{10400}{T(K)}\right]$$

Q. 1. Obtain design Eqn for the process.

2. Since catalyst deactivates, what is the reactor temperature after 30 days.

$$\frac{dF_A}{dV} = r_A$$

$$= k_2 C_B - k_1 C_A$$

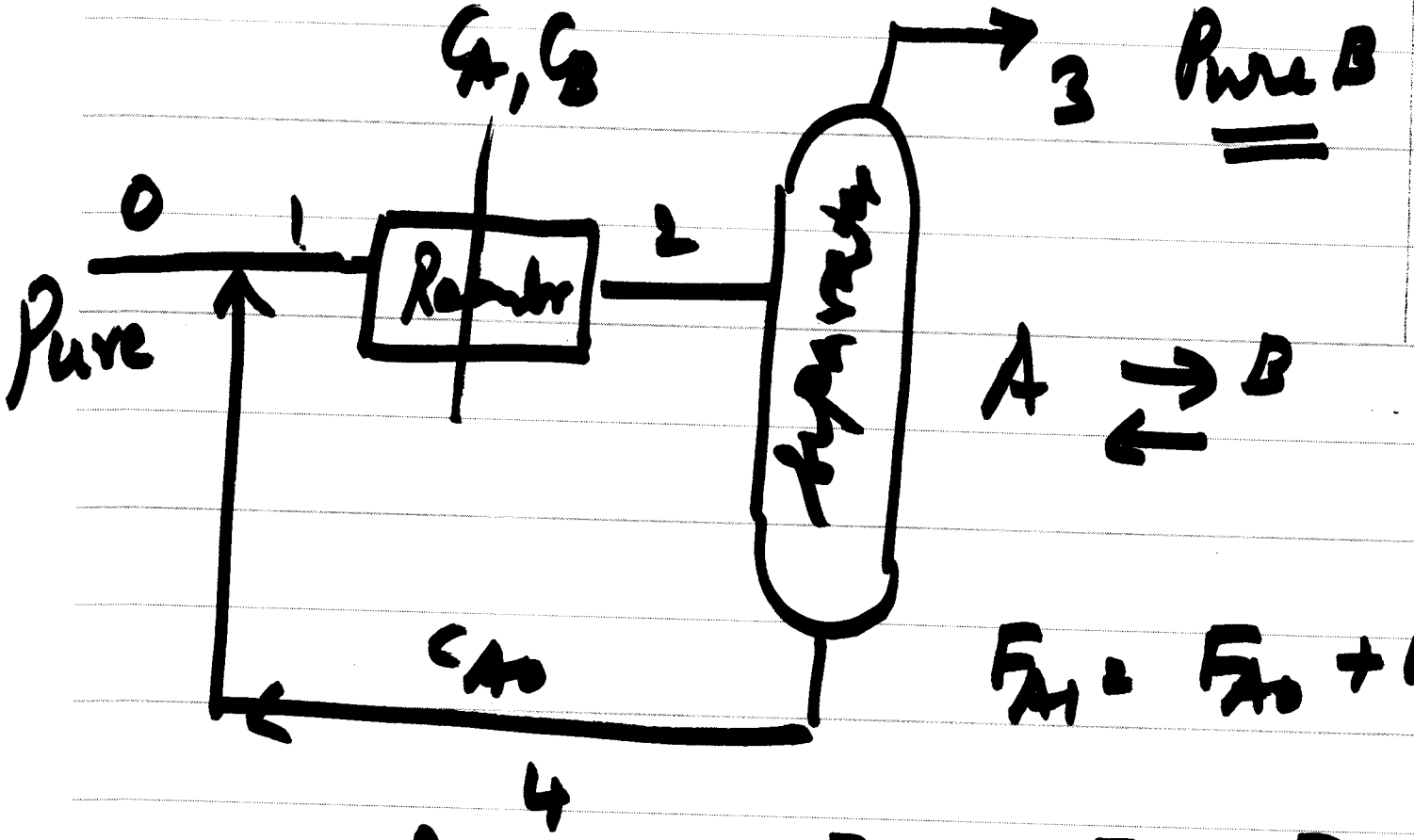
$$-F_{A0}\frac{dx}{dV} = k_2$$

$$F_A =$$

$$F_A = F_{A0}(1-x)$$

$$C_B = \frac{F_A}{v_0}$$

$$C_B = \frac{F_{A0} y_A}{v_0}$$



$F_{A1} = F_{A0} + F_{A4}$

$F_{A1} = F_{A0} + F_{A2} = F_{A0} + F_{A1}(1-y_2)$

y is conversion defined with respect to position '0'

$$F_{A1} = F_{A0} + F_{A4}$$

$$= F_{A0} + F_{A2} = F_{A0} + F_{A1}(1-y_2)$$

$$F_{A1} = F_{A0}/y_2$$

$$C_{A4} = C_{A0}$$

$$v_4 = \frac{F_{A4}}{C_{A4}} = \frac{F_{A2}}{C_{A4}} = \frac{F_{A1}}{C_{A0}}(1-y_2) = \frac{F_{A0}(1-y_2)}{y_2 C_{A0}}$$

$$v_1 = v_0 + v_4 = v_0 + \frac{v_0}{y_2}(1-y_2) = v_0/y_2$$

$$C_A = \frac{F_A}{v} = \frac{F_{A1}(1-y)}{(v_0/y_2)}$$

$$= \frac{\left(\frac{F_{A0}}{y_2}\right)(1-y)}{(v_0/y_2)} = C_{A0}(1-y)$$

$$C_B = C_{A0}\, y$$

$$\frac{dF_A}{dV} = R_A$$

$$-F_{A_0}\frac{dy}{dV} = -k_1 C_{A_0}(1-y) + k_2 C_{A_0} y$$

$$\frac{F_{A_0}}{y_2}\frac{dy}{dV} = k_1 C_{A_0}(1-y) - k_2 C_{A_0} y$$

$$\beta = \left(\frac{K+1}{K}\right)$$

$$\frac{v_0}{y_2}\frac{dy}{dV} = k_1(1-\beta y)$$

$$(k_1)V = -\frac{v_0 \ln(1-\beta y)}{y_2 \beta}$$

(k_1, α)

$$k_d = k_{d_0} \exp(-E_a/RT) \quad - (*)$$

$$-r_A^{(t)} = k(T)\, a(t)\, f(c)$$

$$f(T) = \underbrace{k(T) \exp(-k_d t)}_{= \text{Constant.}} \quad - (**)$$